Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Enhanced reduction of bromate by highly reactive and dispersive green nano-zerovalent iron (G-NZVI) synthesized with onion peel extract

Olga Lem [a], Sunho Yoon [b], Sungjun Bae[b], Woojin Lee [*a]

[a]Department of Civil and Environmental Engineering, National Laboratory Astana, Nazarbayev University, Nur-sultan 010000, Republic of Kazakhstan

[b]Department of Civil and Environmental Engineering, Konkuk University, Seoul 05029, Republic of Korea

*Corresponding author: phone: +7-7172-70-6540

E-mail: woojin.lee@nu.edu.kz

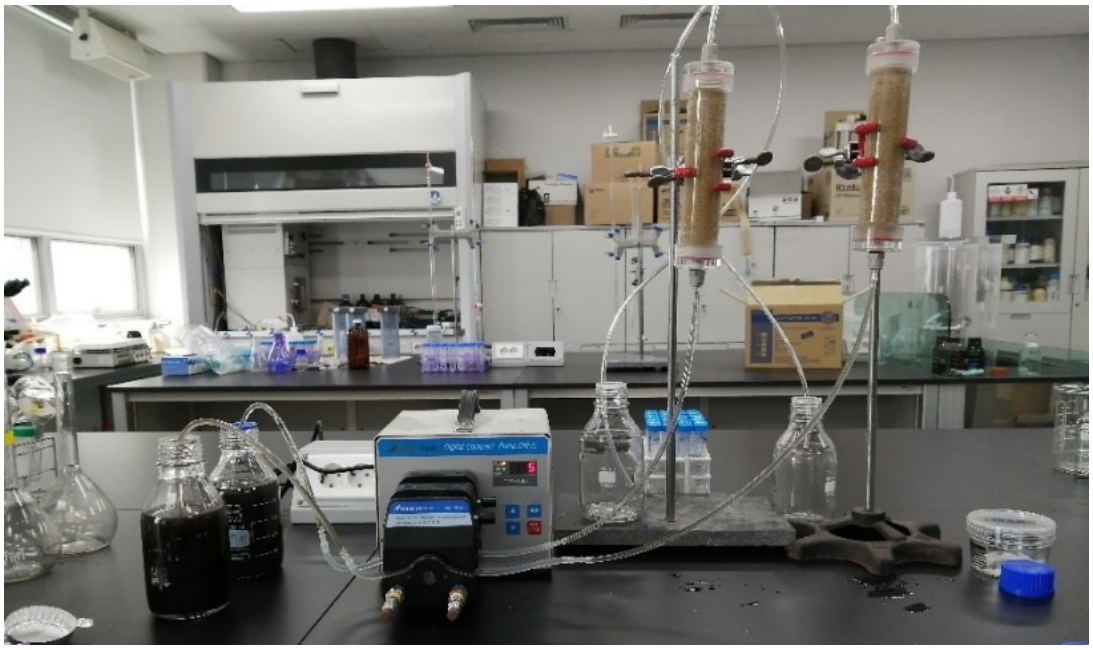

Figure S1. Experimental set up of mobility test

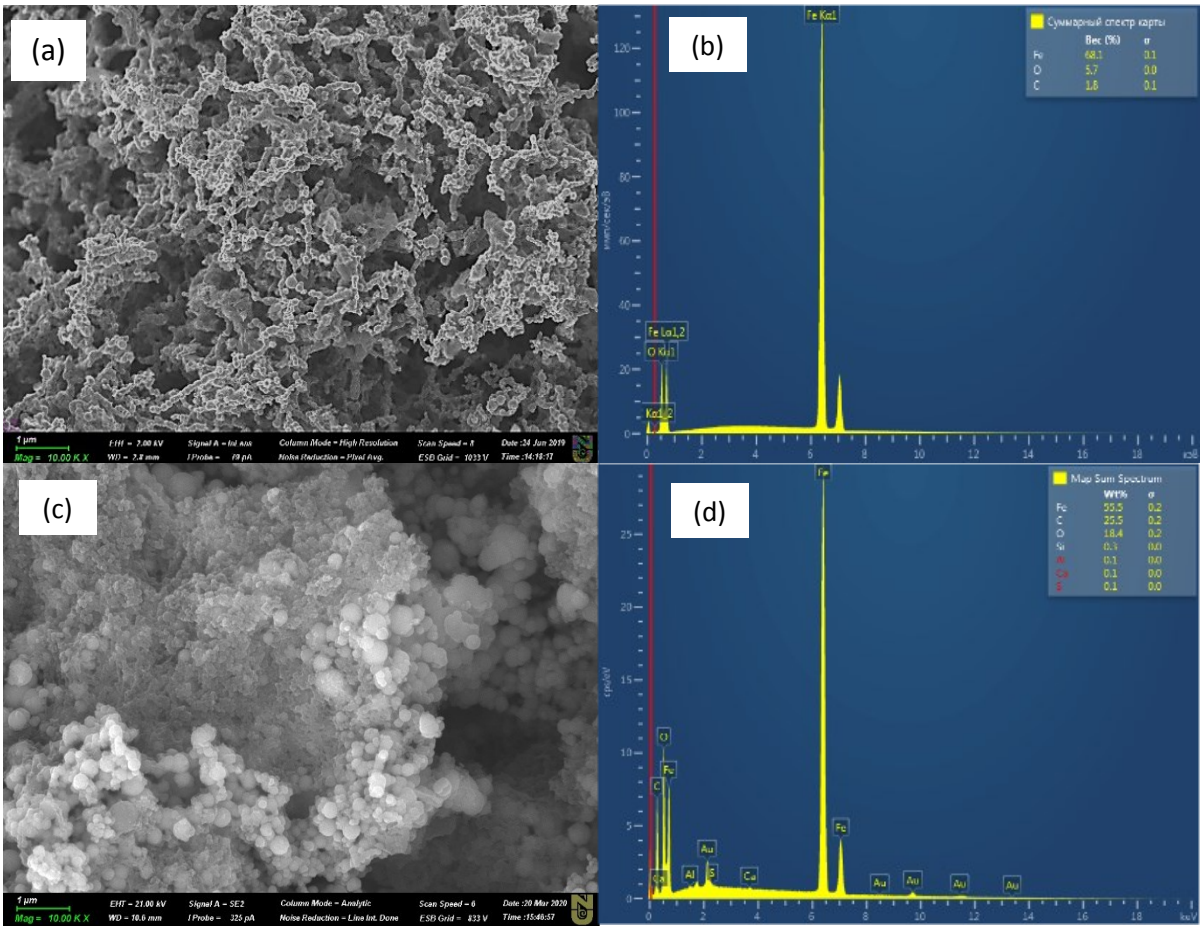

Figure S2. SEM-EDS images of NZVI ((a) and (b)) and G-NZVI ((c) and (d)).

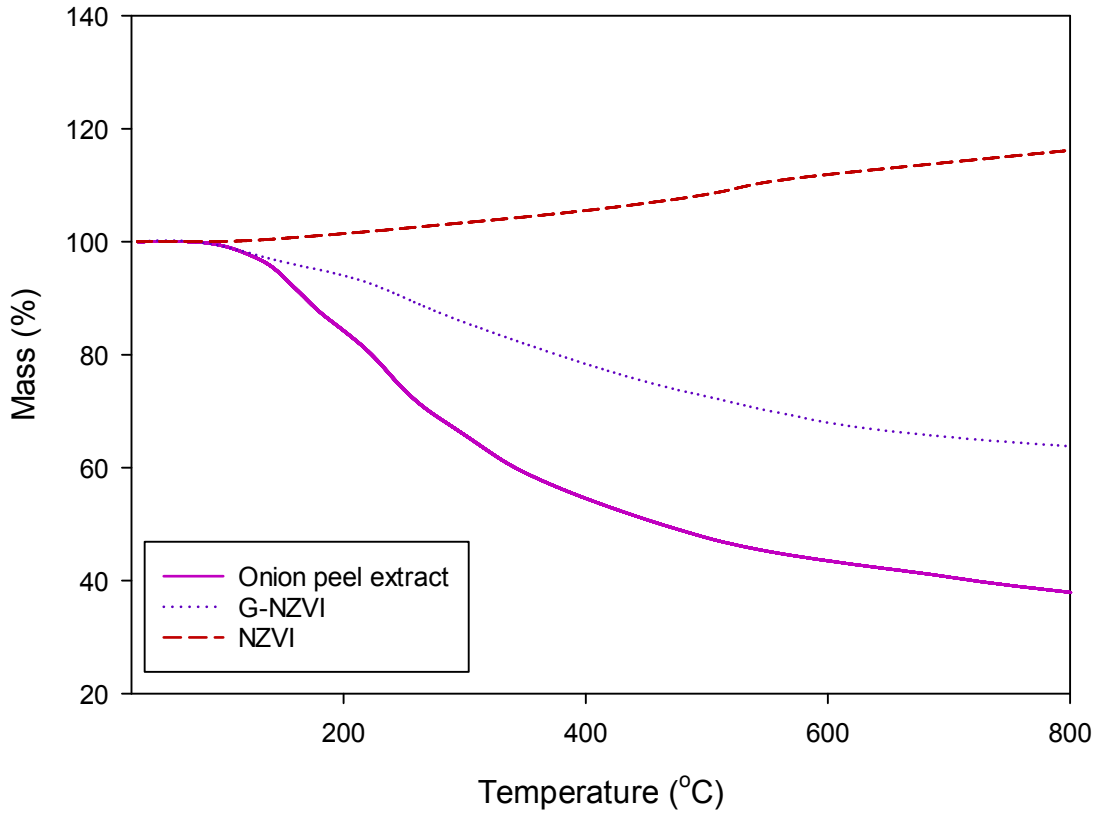

Figure S3. TGA profiles of NZVI, onion peel extract, and G-NZVI.

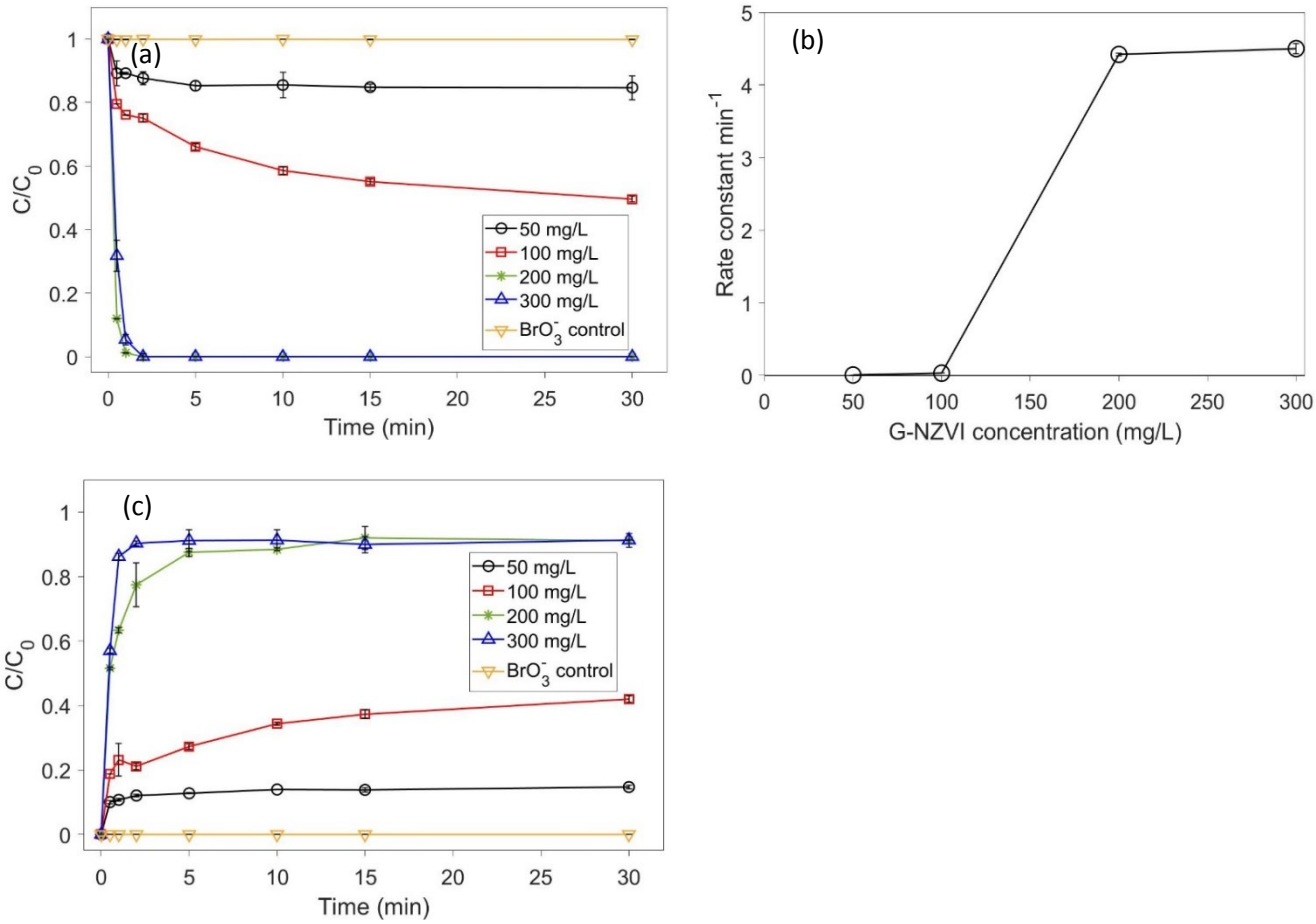

Figure S4. Effect of G-NZVI loading on the removal efficiency of BrO_3^- (50 mg/L) (a), the k_1 values obtained from each suspension (b), and corresponding Br^- formation (c).

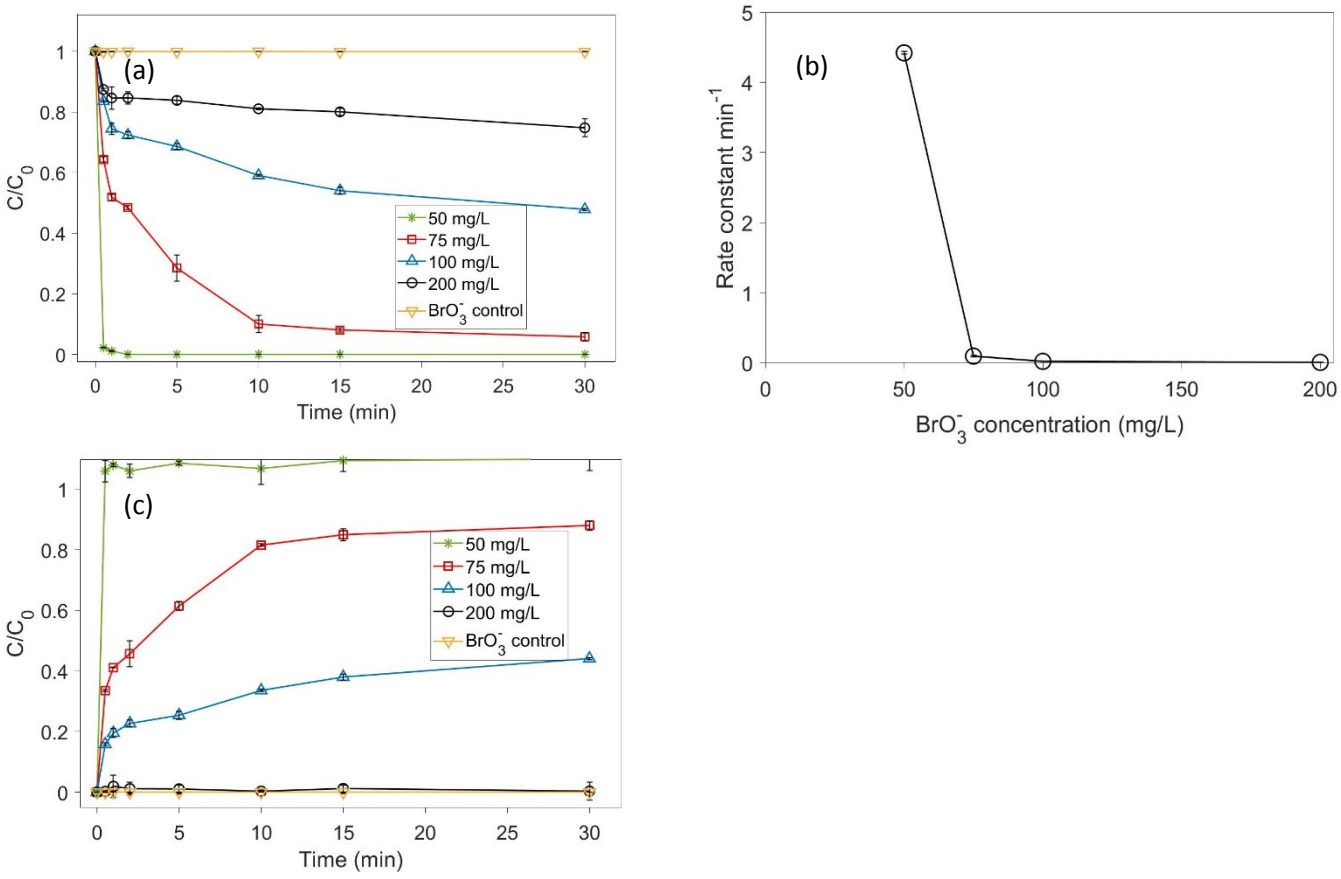

Figure S5. Effect of BrO_3^- concentration on the removal efficiency of BrO_3^- by G-NZVI (a), the k_1 values obtained from each suspension (b), and corresponding Br^- formation (c).

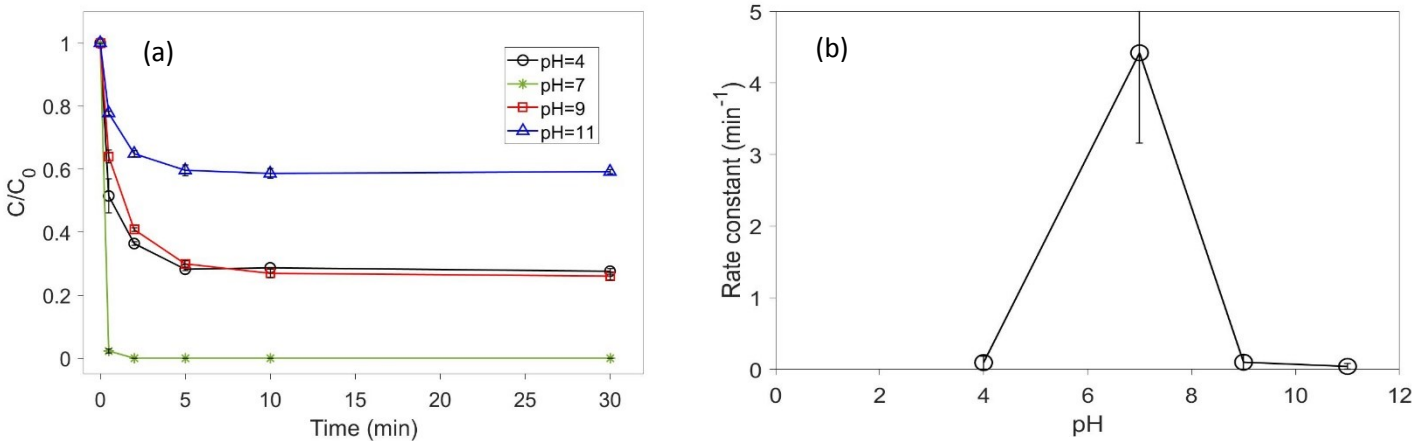

Figure S6. Effect of pH on the removal efficiency of BrO_3^- by G-NZVI (a) and the k_1 values obtained from each suspension (b).

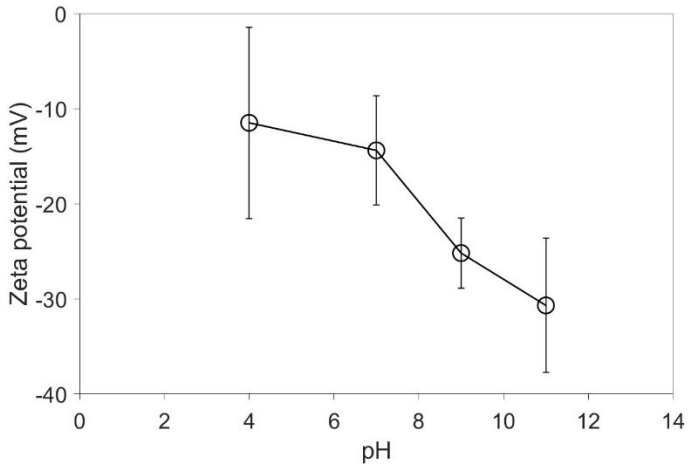

Figure S7. Zeta potential of G-NZVI as a function of pH.

Table S1. Theoretically calculated Gibbs free energy values and spontaneity of reactions

	Polyphenols (0.3-0.8)	BrO_3^-/Br^- (1.478)	Fe^{3+}/Fe^{2+} (0.771)	Fe^{3+}/Fe^0 (-0.037)	Fe^{2+}/Fe^0 (-0.44)
Polyphenols (0.3-0.8)*		ΔG>0, NS**	ΔG<0, S***	ΔG<0, S	ΔG<0, S
BrO_3^-/Br^- (1.478)	ΔG>0, NS		ΔG>0, NS	ΔG<0, S	ΔG<0, S
Fe^{3+}/Fe^{2+} (0.771)	ΔG<0, S	ΔG>0, NS			
Fe^{3+}/Fe^0 (-0.037)	ΔG<0, S	ΔG<0, S			
Fe^{2+}/Fe^0 (-0.44)	ΔG<0, S	ΔG<0, S			

*Potential energy (V)

**NS: non-spontaneous reaction

***S: spontaneous reaction

Table S2. Comparison of kinetic rate constants of pseudo-first-order and second-order reactions

Supporting information

	Pseudo-first-order		Second-order	
G-NZVI loading mg/L	Rate constant (k_1) min^{-1}	R^2	Rate constant (k_2) M/min	R^2
50	0.006	0.43	0.0071	0.42
100	0.0318	0.81	0.0456	0.86
200	4.42	0.98	28.301	0.90
300	4.5	0.96	8.7516	0.85
BrO_3^- loading mg/L	Rate constant (k_1) min^{-1}	R^2	Rate constant (k_2) M/min	R^2
50	4.42	0.98	27.005	0.90
75	0.088	0.78	0.057	0.94
100	0.022	0.81	0.033	0.87
200	0.006	0.85	0.008	0.68